Scalable Nonparametric Sampling from Multimodal Posteriors with the Posterior Bootstrap

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Dirichlet Distribution, definition

Dirichlet distribution: multivariate generalisation of the Beta distribution.

pdf is given by

$$f(x; \alpha) = \frac{1}{B(\alpha)} \prod_{i=1}^{p} x_i^{\alpha_i - 1} \quad (1)$$

where $x \in \mathbb{R}^p, \sum_i x_i = 1$ and $\alpha \in \mathbb{R}^p, a_i > 0$, and $B(\alpha)$ is a normalisation term.

Dirichlet Distribution, visualisation

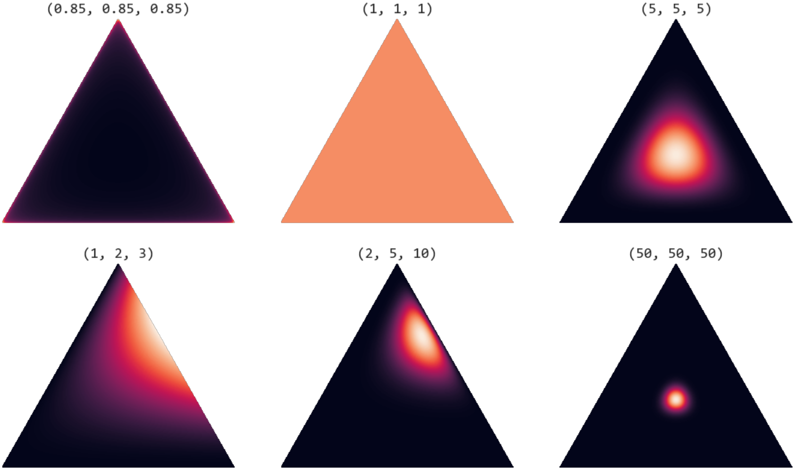


Figure: source:
https://towardsdatascience.com/dirichlet-distribution-a82ab942a879

Dirichlet Processes, definition

Dirichlet Process: a stochastic process where a finite subset of random variables have a Dirichlet distribution.

Dirichlet processes are specified by a base probability distribution, H and a concentration parameter α. Then for some finite disjoint partition of $S = \{B\}_{i=1}^{n}$ we have

$$(X_{B_1}, \ldots, X_{B_n}) \sim \text{Dirichlet}(\alpha H(B_1), \ldots, \alpha H(B_n)) \tag{2}$$

Dirichlet Processes, some intuition

What is a die?

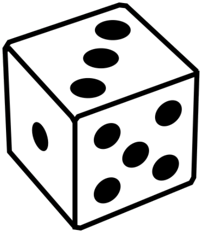
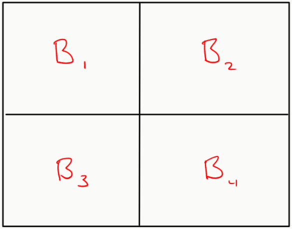


Figure: A Statistician's best friend (sorry coins).

Dirichlet Processes, some intuition

Sampling form a DP has the bi-product of a new probability distribution.

1. Partition a space



2. Compute some parameters

$$\mathrm{Dir}(\alpha H(B_1), \ldots, \alpha H(B_4))$$

3. Sample some weights

$$(X_{B_1}, X_{B_2}, X_{B_3}, X_{B_4})$$

Questions / Comments?

And then we're onto the paper!

Bayesian Non-parametric learning

Let $y = (y_1, \ldots, y_n)$ where $y_i \stackrel{iid}{\sim} F_0$ and let $\theta \in \Theta \subseteq \mathbb{R}^p$ be a parameter that indexes a family of probability distribution $\mathcal{F}_\Theta$.

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Then we are interested in

$$\theta_0(F_0) = \arg\min_\theta \int l(y;\theta) dF_0(y) \tag{3}$$

where $l(y;\theta)$ is a loss function. For example if $l = (y-\theta)^2$ we would recover the mean.

Bayesian Non-parametric learning, cont.

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Put a prior on it

Putting a DP prior on F_0

$$F|a, F_\pi \sim DP(a, F_\pi) \tag{4}$$

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where

$$G_n = \frac{a}{a+n}F_\pi + \frac{1}{a+n}\sum_i \delta_{y_i} \tag{6}$$

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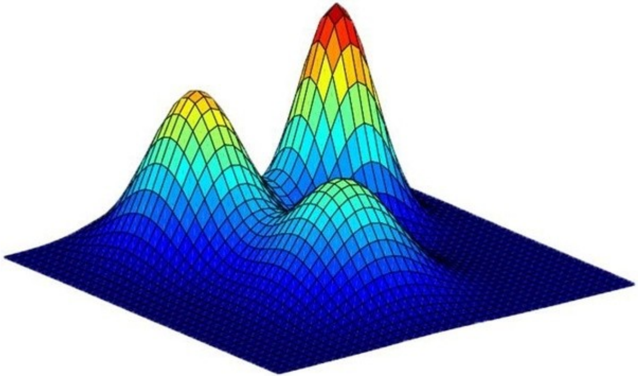
We can sample from $\pi(\theta|y_{1:n})$ using the following algorithm

Algorithm 1 NPL Posterior Sampling

for $i = 1$ **to** B **do**
  Draw $F^{(i)} \sim \mathrm{DP}(\alpha + n, G_n)$
  $\theta^{(i)} = \arg\min_\theta \int l(y, \theta)dF^{(i)}(y)$
end for

Gaussian Mixture Models

Weighted mixture of Gaussians



Gaussian Mixture Models, cont.

To use Bayesian Non-parametric learning all we need to do is define a loss function

$$l(y, \pi, \mu, \sigma) = -\log \sum_{=1}^{K} \pi_k \mathcal{N}(y; \mu_k, \text{diag}(\sigma_k^2)) \tag{8}$$

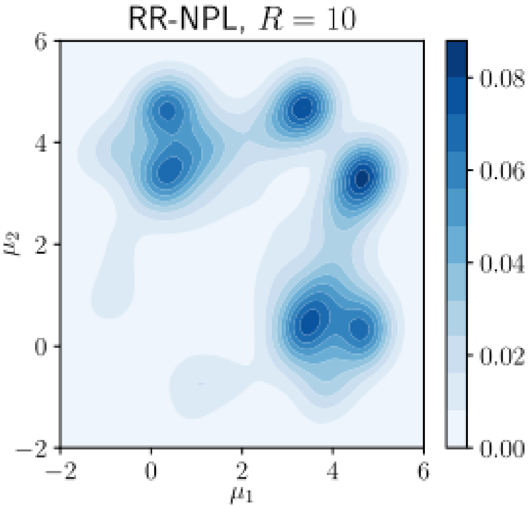
GMMs have multi-modal posteriors.

Gaussian Mixture Models, cont.

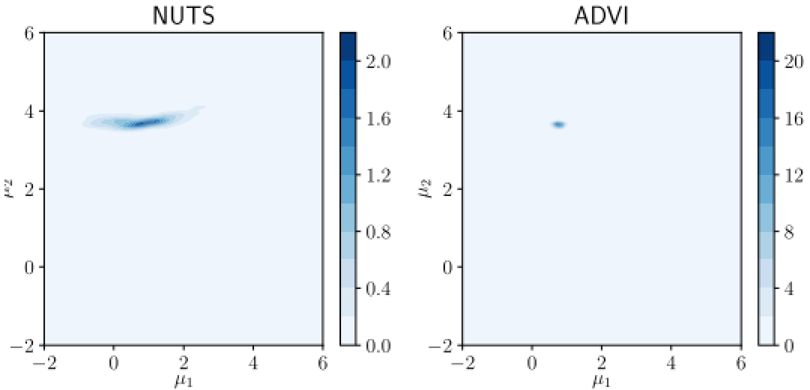
For the example, there are $K = 3$ groups, with

$$\begin{aligned} \pi &= (0.1, 0.3, 0.6) \\ \mu_0 &= (0, 2, 4) \\ \sigma_0^2 &= (1, 1, 1) \end{aligned}$$

Gaussian Mixture Models, cont.



Gaussian Mixture Models, cont.



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No! We might not care about those modes, but getting something useful out of the posterior. It's not really clear how we can do that.

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In practice we need to truncate somewhere But that means we're going to be approximating

$$\pi(\theta|y_{1:n}) = \int \pi(\theta|F) d\pi(F|y_{1:n}) \tag{9}$$

Approximate posterior sampling

Algorithm 2 Posterior Bootstrap Sampling

Define T as truncation limit

Observed samples are $y_{1:n}$

for $i = 1$ **to** B **do**

Draw prior pseudo-samples $\tilde{y}^{(i)}_{1:T} \overset{iid}{\sim} F_\pi$

Draw $(w^{(i)}_{1:n}, \tilde{w}^{(i)}_{1:T}) \sim \mathrm{Dir}\,(1, \ldots, 1, \alpha/T, \ldots, \alpha/T)$

$$\theta^{(i)} = \arg\min_\theta \left\{ \sum_{j=1}^n w^{(i)}_j l(y_j, \theta) + \sum_{k=1}^T \tilde{w}^{(i)}_k l(\tilde{y}^{(i)}_k, \theta) \right\}$$

end for

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Algorithm 4 FI-NPL Posterior Sampling

Select θ^{init} from mode of interest
for $i = 1$ **to** B **do**
  Draw $F^{(i)} \sim \text{DP}(\alpha + n, G_n)$
  $\theta^{(i)} = \text{local arg min}_\theta \left(\int l(y, \theta) dF^{(i)}(y), \theta^{\text{init}} \right)$
end for

Back to GMMs

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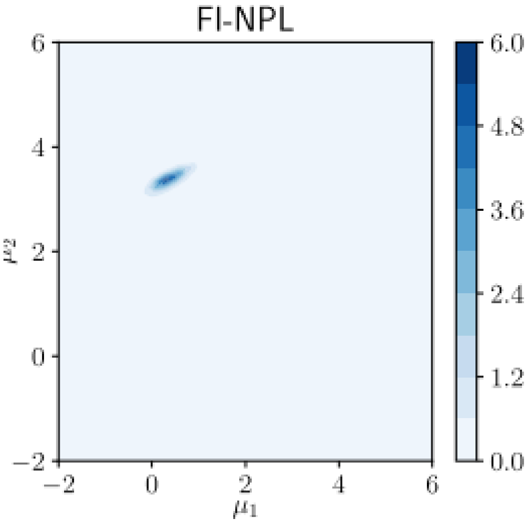


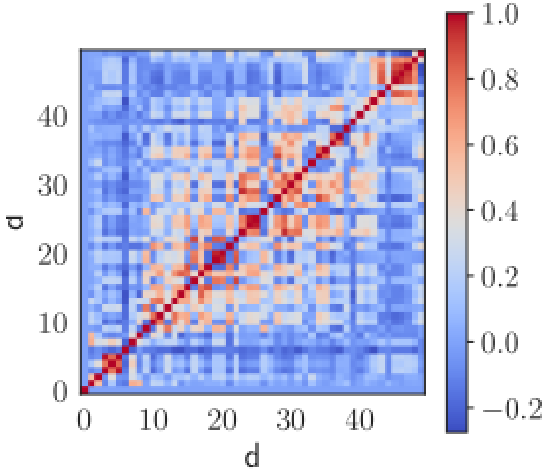
Example #2

Analysis of genotype / psuedo phenotype dataset, where the phenotype was generate by

$$y_i \sim \mathrm{Bernoulli}(\sigma(\beta^\top x_i)) \tag{10}$$

where $\beta \in \mathbb{R}^{50}$ with 5 randomly selected non-zero components.

Correlation Matrix



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So all we need to do is have a sparsity inducing loss function.

$$l(y,\theta) - \log f_\theta(y) + \gamma g(\theta) \tag{11}$$

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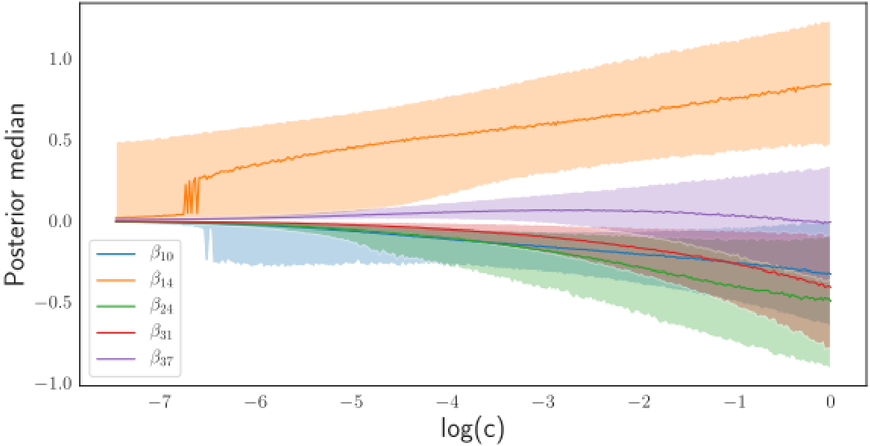
Example: setting $g(\theta) = |\theta|$ gives the Bayesian NPL-Lasso

Example #2, results



Conclusions

A cool idea for uncertainty quantification.

Priors aren't really a thing, it's all done via the loss function

Captures multi-modality

Quick if we have a lot of compute, sampling from the NPL posterior can be done in parallel

Thanks for Listening

Questions?